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A COMPARISON OF CALPUFF MODELING RESULTS TO TWO TRACER FIELD EXPERIMENTS

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1.0 INTRODUCTION

Dispersion models such as the Industrial Source Complex Short Term (EPA, 1995) typically assume steady, horizontally homogeneous wind fields instantaneously over the entire modeling domain and are usually limited to 50 kilometers from a source. However, applications hundreds of kilometers from a source require other models or modeling systems. At these distances, the transport times are sufficiently long that the mean wind fields cannot be considered steady or homogeneous. CALPUFF is one such modeling system, consisting of several components: CALMET, a meteorological preprocessor that utilizes surface, upper air, and on-site meteorological data to create a three-dimensional wind field and derive boundary layer parameters based on gridded land use data; CALPUFF, a puff dispersion model that can simulate the effects of temporally and spatially varying meteorological conditions on pollutant transport, remove pollutants through dry and wet deposition processes, and transform pollutant species through chemical reactions; and CALPOST, a postprocessor that takes the hourly estimates from CALPUFF and generates *n*-hr estimates as well as tables of maximum values.

Concentration estimates from the CALPUFF dispersion model were compared to observed tracer concentrations from two short term field experiments. The first experiment was at the Savannah River Laboratory (SRL) in South Carolina in December 1975 (DOE, 1978) and the second was the Great Plains experiment near Norman, Oklahoma (Ferber et al., 1981) in July 1980. Both experiments examined long-range transport of inert tracer materials to demonstrate the feasibility of using other tracers as alternatives to the more commonly used sulfur hexafluoride (SF_6). Several tracers were released for a short duration (3-4 hours) and the resulting plume concentrations were recorded at an array of monitors downwind from the source. For the SRL field experiment, monitors were located about 100 kilometers from the source. For the Great Plains experiment, arcs of monitors were located 100 and 600 kilometers from the source.

Previous studies have compared the results from the Great Plains experiment to dispersion model results. Carhart et al. (1989) intercompared the results from eight short-term, long-range dispersion models to the Great Plains results and to a longer-term study at the Savannah River Laboratory (not the same as used in this study). The primary method for evaluating model performance was the use of the American Meteorological Society (AMS) statistical measures (Fox, 1981) and graphical techniques. They concluded that model results compared in space and in time to observations were generally poor and that predictions for a specific location and time for averaging periods less than one day were not reliable. They also noted that unpairing decreases the scatter. They concluded that "model improvement can be made by better representing the wind field. The use of multiple layers seems to improve results substantially."

The transport and diffusion of a tracer gas was simulated by Moran and Pielke (1995a,b) using the Colorado State University mesoscale atmospheric dispersion modeling system, which consists of a prognostic meteorological model coupled to a mesoscale Lagrangian particle dispersion model. Results from several simulations with the model were compared to observations from the Great Plains experiment. Their baseline simulation generally compared favorably to observations for both arcs although directional errors were apparent by up to 20°. The results also suggest that the nocturnal low-level jet plays an important role in transport and

deformation of the tracer plume and that some flow regimes require better temporal resolution of boundary layer winds than is available from the National Weather Service (NWS) twice-daily rawinsondes.

In a study using the CALPUFF dispersion model, Irwin (1997) compared model concentration estimates to observed concentrations at three arcs (3.2, 48, and 90 kilometers) of monitors downwind of a three-hour tracer release in April 1977 near Idaho Falls, ID. The primary focus in Irwin's analysis was the characterization of transport and dispersion using different combinations of surface and upper air data. He found that the lateral dispersion was best characterized when all the meteorological data were used but the location of the simulated maximum relative to the observed maximum on each arc was poorly characterized regardless of the data used.

In this report, the CALPUFF modeling domains, the meteorological data, terrain and land use data, sources, receptors and modeling options are described in Sections 2 through 7. Analyses and discussions are presented in Section 8. Irwin's paper is presented in its entirety in Appendix A.

2.0 MODELING DOMAIN

The CALPUFF modeling system uses a grid system consisting of an array of horizontal grid cells and multiple vertical layers. Two grids must be defined in the CALPUFF model -- meteorological and computational. The meteorological grid defines the extent over which land use, winds, and other meteorological variables are defined. The computational grid defines the extent of the concentration calculations, and is required to be identical to or a subset of the meteorological grid. For the SRL and Great Plains simulations, the computational grid is defined to be identical to the meteorological grid. A third grid, the sampling grid, is optional and is used to define a rectangular array of receptor locations. The sampling grid must be identical to or a subset of the computational grid. It may also be nested inside the computational grid, i.e., several sampling grid cells per computational grid cell. For these applications, a sampling grid identical to the computational grid was used with a nesting factor of one (sampling grid cell size equal to the cell size of the computational grid).

To properly characterize the meteorology for the CALPUFF modeling system, a grid that spans, at a minimum, the distance between source and receptor is required. However, to allow for possible recirculation of puffs that may be transported beyond the receptors and to allow for upstream influences on the wind field, the meteorological and computational domains should be larger than this minimum.

For the Savannah River Laboratory (SRL) field experiment, a meteorological grid extending from 32° N to 34° N latitude and from 80° W to 82° W longitude was used. Figure 1 shows the region of the SRL field experiment. The SRL facility is near the west edge of the domain and the sampling monitors are located along Interstate 95. The distance between the source and the receptors is approximately 100 kilometers. A 24-by-24 horizontal grid with a 10-kilometer resolution was used for the SRL modeling.

The Great Plains site is shown in Figure 2. Two arcs of monitors were deployed during the field experiment -- 100 and 600 kilometers. For this analysis, two separate grids were defined. For the 100-kilometer arc, a grid extending approximately from 35° N to 36.5°N latitude and from 96° W to 98.5° W longitude was defined. A 42-by-40 horizontal grid with a 10-kilometer resolution was used for this arc. For the 600-kilometer arc, the grid extended from approximately 35° N to 42°N latitude and from 89° W to 100° W longitude. A 44-by-40 horizontal grid with a 20-kilometer resolution was used for this arc.

To adequately characterize the vertical structure of the atmosphere, six layers were defined: surface-20, 20-50, 50-100, 100-500, 500-2000, and 2000-3300 meters. This vertical resolution is consistent with the analysis by Irwin (1997) of the 1977 Idaho Falls field study.

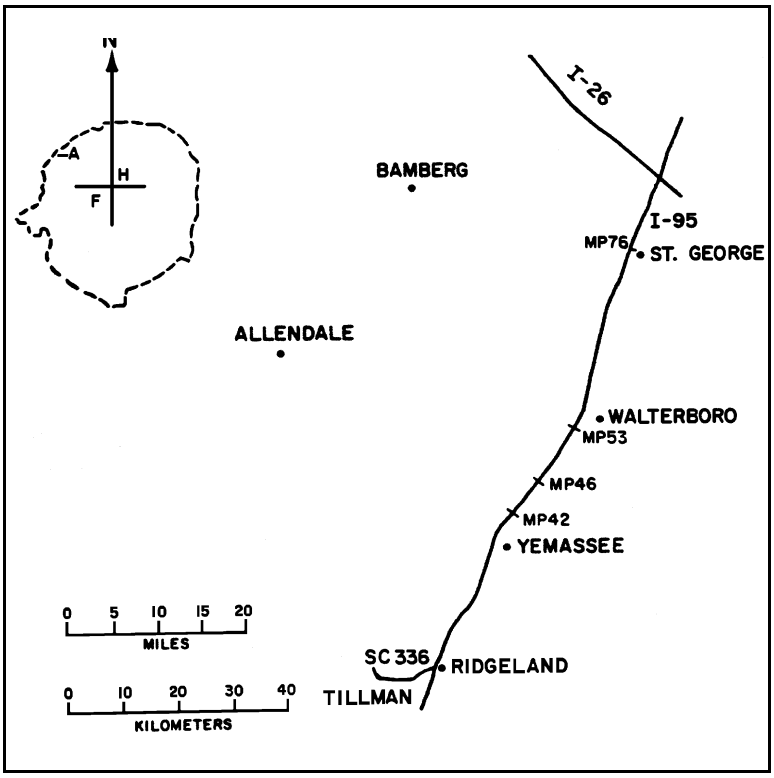

Figure 1. Savannah River Laboratory field experiment site.

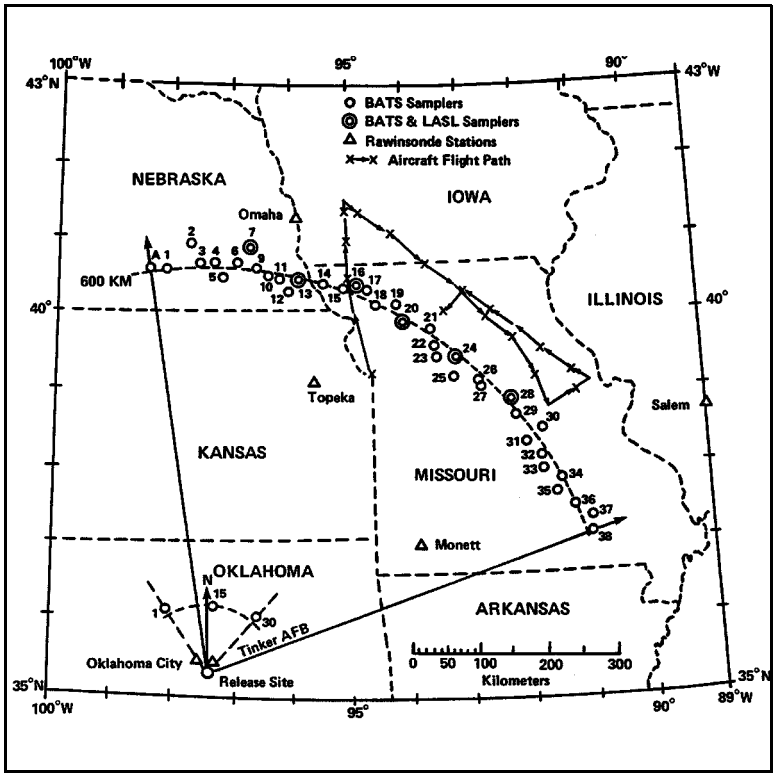

Figure 2. Great Plains field experiment site.

3.0 METEOROLOGICAL DATA

The CALMET preprocessor utilizes NWS meteorological data and on-site data to produce temporally and spatially varying three dimensional wind fields for CALPUFF. Only NWS data were used for this effort and came from two compact disc (CD) data sets (information on where to obtain these discs is in Appendix B). The first was the *Solar and Meteorological Surface Observation Network* (SAMSON) compact discs, which were used to obtain the hourly surface observations. The following surface stations were used for each of the field experiments:

Savannah River Laboratory

Georgia:	Athens, Atlanta, Augusta, Macon, Savannah
North Carolina:	Asheville, Charlotte, Greensboro, Raleigh-Durham, Wilmington
South Carolina:	Charleston, Columbia, Greer-Spartanburg

Great Plains

Arkansas:	Fort Smith
Iowa:	Des Moines
Illinois:	Springfield
Kansas:	Dodge City, Topeka, Wichita
Missouri:	Columbia, Kansas City, Springfield, St. Louis
Nebraska:	Grand Island, Omaha, North Platte
Oklahoma:	Oklahoma City, Tulsa
Texas:	Amarillo, Dallas-Fort Worth, Lubbock, Wichita Falls

Twice daily soundings came from the second set of compact discs, the *Radiosonde Data for North America*. The following stations were used for each of the field experiments:

Savannah River Laboratory

Georgia:	Athens, Waycross
North Carolina:	Greensboro, Cape Hatteras
South Carolina:	Charleston

Great Plains

Arkansas:	Little Rock	Nebraska:	North Platte, Omaha
Illinois:	Peoria	Oklahoma:	Oklahoma City
Kansas:	Dodge City, Topeka	Texas:	Amarillo
Missouri:	Monett		

4.0 TERRAIN AND LAND USE DATA

CALMET requires a file of terrain elevations and geophysical parameters in order to prepare the wind fields and other meteorological parameters. The geophysical parameters are derived from geographical information system (GIS) land use categories. Terrain and land use data are available on the CALMET, CALPUFF, and CALPOST Modeling System (version 1.0) CD (hereafter referred to as the CALPUFF CD). Information on obtaining this compact disc is in Appendix B.

The terrain and GIS land use data on the CALPUFF CD were used to define gridded land use data for each field experiment. These data are defined with a resolution of 1/6° latitude and 1/4° longitude. The program PRELND1.EXE, also provided on the CD, was run to extract the data from the GIS data base and map the data to the meteorological domain for each field experiment. The program ELEVAT.EXE (also provided on the CD) was used to process the raw terrain data into average gridded terrain data. The file of terrain and geophysical parameters required by CALMET was constructed from the output files generated by ELEVAT and PRELND1 with additional required records inserted manually to create the final forms of the file for each field experiment.

5.0 SOURCE CHARACTERIZATION

The primary purpose of the Great Plains (Oklahoma) experiment was to demonstrate the efficacy of perfluorocarbons as tracers in atmospheric dispersion field studies. Perfluoromonomethylcyclohexane (PMCH), perfluorodimethylcyclohexane (PDCH), SF_6, and two heavy methanes were released during this experiment. For this analysis, the PDCH emission rates were used since the monitoring data appeared to have a more complete record of PDCH concentrations.

During the Savannah River Laboratory (SRL) study, SF_6 and two heavy methanes were released. For this analysis, the SF_6 tracer emission rates were used. The following source parameters were used for this analysis:

Source	Release height (m)	Stack diameter (m)	Exit velocity ($m\ s^{-1}$)	Exit temp. (K)	Total tracer released (kg)	Length of release (hr)	Emission rate ($g\ s^{-1}$) and tracer
SRL	62.0	1.0*	0.001	ambient	154	4.0	10.69 SF6
Oklahoma (July 8)	10.0	1.0*	0.001	ambient	186	3.0	17.22 PDCH
Oklahoma (July 11)	10.0	1.0*	0.001	ambient	26	3.0	2.41 PDCH

* The stack diameter for each study is the same as was used for the study with the INEL data

For both experiments, the emission rate was assumed to be constant over the entire period of the release. The emission rates were computed as follows:

$$\frac{total\ tracer\ released\ in\ kg}{length\ of\ release\ in\ hours} \times \frac{1000g}{1\ kg} \times \frac{1\ hr}{3600\ \text{sec}}$$

The exit temperature is assumed to be the same as the ambient atmospheric temperature. CALPUFF checks the difference between the stack exit temperature and the surface station temperature. If this difference is less than zero, the difference is set to zero. To insure this condition, an exit temperature of 250 K was input to the model.

6.0 RECEPTORS

Both discrete and gridded receptors were used in this study. The discrete receptors were placed at approximately the same distance as the monitoring arcs. The gridded receptors were located at the center of each sampling grid cell to provide sufficient information to plot contours of concentration estimates.

For the SRL experiment, a single monitoring arc was used at approximately 100 kilometers. The monitors were located along I-95 (Figure 1) from Mile Post 76 (MP76) on I-95 near St. George, SC south to Hwy 336 west of Tillman, SC and along SC 336. The monitors subtended an arc of about 70°. Receptors for modeling were placed along an arc every 1/4° degree from MP76 to MP22 near Ridgeland, resulting in 261 receptor locations. The distance between receptors was about 440 meters.

For the July 8 Great Plains experiment, there were two arcs of monitors: 100 kilometers and 600 kilometers as shown in Figure 2. At 100 kilometers, the monitors subtend an arc of about 75°. Receptors were placed every 1/4° degree, extending beyond the edges of the monitoring arc, resulting in 361 receptor locations. The distance between receptors was about 440 meters. At the 600-kilometer arc, the monitors subtend an arc of about 80°. Receptors were placed every 1/2° degree, about every 5,200 meters apart, resulting in 161 receptor locations.

7.0 MODELING OPTIONS

In the CALPUFF modeling system, each of the three programs (CALMET, CALPUFF, and CALPOST) uses a control file of user-selectable options to control the data processing. There are numerous options in each and several that can result in significant differences. The following model controls for CALMET and CALPUFF were employed for the analyses with the tracer data.

7.1 CALMET Options

The following CALMET control parameters and options are chosen to be consistent with the 1977 INEL study by Irwin (1997). The most important options relate to the development of the wind field and were set as follows:

IWFCOD	= 1	Use diagnostic wind model to develop the 3-D wind fields
IFRADJ	= 1	Compute Froude number adjustment effects (thermodynamic blocking effects of terrain)
IKINE	= 1	Compute kinematic effects of terrain
IOBR	= 0	Do NOT use O'Brien procedure for adjusting vertical velocity
IEXTRP	= 4	Use similarity theory to extrapolate surface winds to upper layers
IPROG	= 0	Do NOT use prognostic wind field model output as input to diagnostic wind field model

Mixing heights are important in the estimating ground level concentrations. The options that affect mixing heights were set as follows:

IAVEZI	= 1	Conduct spatial averaging
MNDAV	= 3	Maximum search radius (in grid cells) in averaging process
HAFANG	= 30.	Half-angle of upwind looking cone for averaging
ILEVZI	= 1	Layer of winds to use in upwind averaging
DPTMIN	= .001	Minimum potential temperature lapse rate (K/m) in stable layer above convective mixing height
DZZI	= 200	Depth of layer (meters) over which the lapse rate is computed
ZIMIN	= 20	Minimum mixing height (meters) over land
ZIMAX	= 3300	Maximum mixing height (meters) over land, defined to be the top of the modeling domain

7.2 CALPUFF Options

The following CALPUFF control parameters, which are a subset of the control parameters, were used. As with CALMET, these parameters and options were chosen to be consistent with the 1977 INEL study.

Technical options (group 2):

MCTADJ	= 0	No terrain adjustment
MCTSG	= 0	No subgrid scale complex terrain is modeled
MSLUG	= 1	Near field puffs modeled as elongated (i.e., slugs)
MTRANS	= 1	Transitional plume rise is modeled
MTIP	= 1	Stack tip downwash is modeled
MSHEAR	= 0	Vertical wind shear is NOT modeled above stack top
MCHEM	= 0	No chemical transformations
MWET	= 0	No wet removal processes
MDRY	= 0	No dry removal processes
MPARTL	= 0	No partial plume penetration
MREG	= 0	No check made to see if options conform to regulatory options

Two different values were used for the option MDISP:

	= 2	Dispersion coefficients from internally calculated sigmas
	= 3	PG dispersion coefficients for RURAL areas

Several miscellaneous dispersion and computational parameters (group 12) were set as follows:

SYTDEP	= 550.	Horizontal puff size beyond which Heffter equations are used for sigma-y and sigma-z
MHFTSZ	= 0	Do NOT use Heffter equation for sigma-z
XMXLEN	= 0.1	Maximum length of slug (in grid cells)
XSAMLEN	= 0.1	Maximum travel distance of puff/slug (in grid cells) during one sampling step
MXNEW	= 199	Maximum number of slugs/puffs released during one time step
SL2PF	= 5.0	Slug-to-puff transition criterion factor (= sigma-y/slug length)

8.0 ANALYSIS OF THE CALPUFF CONCENTRATION ESTIMATES

With field experiment results, where data are collected at arc(s) of monitors for short periods of time, the standard statistical measures to compare observed and estimated concentration data, such as recommended by the American Meteorological Society (Fox, 1981), are not easily interpreted. One way to present the results is to compare "n-hour" averages, where "n" represents the time required for the plume to pass the arc of receptors. Measures that can be used to compare results include the fitted and absolute (centerline maximum concentration (Cmax and Omax), the lateral dispersion, σ_y, and the crosswind integrated concentration (CWIC) for the observed concentration and the model estimates. Additionally, the time required for the plume to reach the arc, the length of time required to pass the arc, and the location of the plume centerline can provide information on how well a model simulated the plume transport. These measures with graphical displays of the data are used here to present the results.

Using the Colorado State University (CSU) mesoscale atmospheric dispersion (MAD) model, Moran and Pielke (1995a,b) simulated the transport and dispersion of the tracer cloud for the July 8 Great Plains experiment. The results from his baseline model run (referred to as run 4b in his papers) are included in this analysis. Since they were interested in mesoscale dispersion on the 500-1000 kilometer scale, Moran and Pielke did not simulate the July 11 Great Plains experiment.

The first part of the CSU MAD modeling system consists of the CSU Regional Atmospheric Modeling System (RAMS), a prognostic mesoscale meteorological model that develops three-dimensional mean wind and turbulence fields over complex terrain. A complete description of the RAMS model can be found in Moran and Pielke (1995a). For their simulations, Moran and Pielke (1995a) used a 41 x 46 horizontal grid with a 1/2° longitude by 1/3° latitude resolution and 29 vertical layers. The layer at the surface was 50 meters deep and the domain was extended to 16.2 kilometers using a "1.15 stretch factor." Also included was an 11-level soil model extending to a depth of 0.5 meters.

Table 1 shows the time the plume reached the receptor arc, the length of time for the plume to pass the arc completely, and the plume centerline location based on a fitted curve through the concentration values at each monitor or receptor. Table 2 shows the statistical measures used in the comparison. Two separate CALPUFF model runs were made: 1) using Pasquill-Gifford (P-G) dispersion parameters, and 2) using dispersion coefficients from internally-calculated σ_v and σ_w from the micrometeorological variables calculated in CALMET (hereafter referred to as similarity dispersion). The central maximum concentration is estimated from a Gaussian fit to the modeled and observed data (Cmax) and computed from the CWIC and σ_y, as $C_{max} = CWIC/((\sqrt{2\pi})\sigma_y)$. O_{max} is the actual maximum obtained directly from the monitored and modeled concentrations. The CWIC was computed by trapezoidal integration. The program that computed these measures utilized only those values that were 1% or greater of O_{max}.

8.1 Savannah River Laboratory

The observed concentrations are the cumulative concentration from bag samples located along Interstate 95 from about St. George south to Ridgeland (Figure 1). Background

concentration was estimated to be with a 0.5 part per trillion (ppt) (DOE, 1978). A continuous tracer release started at 1025 Local Standard Time (LST) and continued until 1425 LST. The bag samplers were started at different times, ranging from about 1040 to 1230 LST, and the duration of the sampling ranged from 7.0 to 7.5 hours. Since the release started as 1025 LST, it seems likely that sampling at the monitors would have begun prior to the arrival of the plume at all of the monitors. The arrival time of the modeled plume was the hour ending at 1300 LST for both P-G and similarity dispersion. The simulated plume required seven hours to pass the arc with the P-G dispersion coefficients, but only six hours with similarity dispersion coefficients. Therefore, seven-hour-average modeled and observed concentrations were computed for the Savannah River Laboratory field experiment. Since the first monitors were turned on prior to 1100 LST and only cumulative concentration is reported for the observed data, the simulated concentrations were summed over the seven-hour period from 1100 LST through 1800 LST.

Figure 3a shows the plots of the concentration estimates at the receptors (continuous curves) and the observed concentrations at the receptors (labeled points). The modeled peaks are 10° to 20° further to the south than the observed peak. Figure 3b shows the same plot except the observed concentrations have been shifted by 17° to more closely align with the P-G dispersion simulated concentrations. Clearly, there is general agreement in the shape and magnitude of the distributions.

Note that there are two local maxima in the observations near 135° and 145°. The winds were more northerly shortly after the release and may have resulted in the observed local peaks (DOE, 1978) that were not captured in the modeled meteorology. The observed lateral dispersion is 50-100% larger than the modeled dispersion due to these local peaks (Table 1). If these two secondary peaks are omitted from the analysis, then the statistical measures of the simulated plumes are in better agreement with the measures of the observed plume. Without these secondary peaks, the fitted central maximum to the observations increases by 37% to 3.758 ppt (modeled: PG 7.2 ppt and Similarity 5.1 ppt), σ_y is reduced by 33% to 7.77 km (modeled: PG 6.9 km and Similarity 5.0 km), and the CWIC is reduced only slightly to 0.732 ppt-m (modeled: PG 1.29 ppt-m and Similarity 0.8 ppt-m). The meteorology, as simulated for the Savannah River tracer release, did not characterize this initial difference in wind direction sufficiently to transport the plume more toward the south.

8.2 Great Plains

Two study days in 1980 - July 8 and July 11 - formed the Great Plains tracer experiment. Moran and Pielke, (1995a,b) in their analyses with the CSU MAD model, studied the July 8 case. Results from their baseline simulation are included here for comparison, though he simulated the PMCH release. Moran and Pielke's simulated PMCH concentrations were divided by 1.18 for comparison to the observed and simulated PDCH concentrations. This value is the volume of PMCH divided by the volume of PDCH, as given by Ferber et al. (1981).

8.2.1 July 8, 1980

Beginning at 1300 LST, the PDCH and PMCH tracer gases were released at a constant rate for a three-hour period from an open field at the National Severe Storms Laboratory in Norman, Oklahoma. The PDCH was released at an average rate of 17.22 g s^{-1} as an aerosol spray. Two arcs of air samplers recorded the passage of the tracer plume for this release - the first at 100 kilometers and the second at 600 kilometers. The locations of the samplers at these two arcs are shown in Figure 2. A background concentration for PDCH of 26 ppt (Ferber et al., 1981) was removed from the observed concentrations. The results for the 100-kilometer arc are discussed first.

100 kilometers

The samplers were set to operate for ten 45-minute periods, sufficient time for the tracer material to pass the 100-kilometer arc. The initial sampling period began at 1500 LST, but the concentrations in the first 45-minute period were near the background concentration. The sampling continued through 2230 LST on July 8, with background concentrations observed for the periods after 2100 LST (9th 45-minute period). Near-background concentrations (0-6 ppt depending on the receptor) were observed for the periods 7 and 8 (from 1930 to 2100 LST). Thus, the length of time the plume passed the arc was approximately five hours (1545-2100 LST). The simulated CALPUFF plume using the P-G dispersion coefficients was evident at the 100-kilometer arc for six hours, but the plume passed the arc in five hours when the similarity dispersion coefficients were used (Table 1). Given the transit time of the observed plume and the simulated transit time using similarity dispersion, five-hour average concentrations were used in the analysis. The hours ending 17 through 21 were used to construct the simulated five-hour concentration average (representing the period 1600-2100), and the seven 45-minute periods from 1545 through 2100 LST were used to construct the observed average concentrations.

Moran and Pielke (1995b) used a transit time of 3.75 hours based on near-background concentrations of PMCH recorded for the 7th 45-minute period and later, i.e., five 45-minute periods were used. This difference demonstrates the variability in how to define the plume transit time, and applies to defining the plume width as well. Moran and Pielke (1995a) discuss the arbitrariness of defining plume width and this discussion can be extended to plume transit time past an arc of monitors (the longitudinal dimension of the wind). There are several methods for defining the plume width, and by extension, the transit time (with background removed):

- concentrations above a percentage of the maximum concentration in the interior of the plume, e.g., 10% or 1%,
- a concentration above a threshold that is independent of the plume interior concentrations, e.g., 0.002 or 0.003 ppt above background, and
- nonzero concentrations above background.

The transit time in this analysis is defined by nonzero concentrations with background removed (the third criterion), but the statistical measures were computed only for concentrations greater than 1% of the maximum (the first criterion). Moran and Pielke utilized the second

criterion, with a minimum of 0.003 ppt (without background) as an absolute minimum. The differences in defining the transit time should not alter the conclusions of this analysis.

The five-hour average modeled and observed concentrations for the 100-kilometer arc on July 8 of the Great Plains field experiment are shown in Figure 4a along with Moran and Pielke's baseline simulation (experiment 4b). Two things are immediately apparent: the monitoring did not capture the entire plume and the observed maximum concentration is very likely less than the simulated maxima. Given the incomplete sampling of the observed plume at 100 kilometers for this release, the statistical measures of the observed plume likely are suspect and are not sufficient to draw conclusions regarding model performance. Nonetheless, the measures were calculated for the observed plume and are shown in Table 2 along with the statistics for the simulated plumes and for Moran and Pielke's July 8 simulation.

Although σ_y shows good agreement between simulated and observed plumes in Table 2, from Figure 4a it appears that the lateral dispersion of the observed plume is wider than the dispersion of the simulated plumes. From the available data, the peak may have occurred at or near receptor 12. Aircraft samples suggest that the plume did not extend much more to the west of receptor 12 (Ferber et al., 1981). The agreement between ground level concentrations and aircraft observations taken between 1630 LST and 1800 LST about 1250 meters above the arc of receptors (Figure 11 in Ferber et al., 1981) suggests a well-mixed layer through this depth. With this information, the ground level plume was extended to the west, assuming 0.9 ppt at receptor 10 (azimuth -10°) and 0.0 ppt at receptor 8 (azimuth -15°). The statistical measures for this 'extended' plume are Cmax = 1.3 ppt, σ_y = 10.9 km, and CWIC = 0.35 ppt-m.

Assuming a well-mixed boundary layer (which appears to be a reasonable assumption here based on aircraft observations), the CWIC can be approximated by $Q/(u \bullet z_i)$, where u is wind speed (meters/second) and z_i is the mixing height (meters). From the afternoon sounding for Oklahoma City on this day (not shown), the observed mixing height is about 2500 m with an average wind speed through the boundary layer of about 10 m s^{-1}. The emission rate was 17.22 g s^{-1} for three hours with sampling at the monitors for five hours. These values yield a CWIC of 0.27×10^5 ppt-m, which is slightly smaller than the observed CWIC of 0.29×10^5 ppt-m. However, the modeled boundary layer does not appear to be well-mixed for most hours when the plume is passing the 100-kilometer arc. The modeled mixing heights are around 2000 meters, but σ_z is around 1000 meters between the source and the receptor locations, suggesting that the simulated atmosphere may be neutral, or possibly stable. These conditions would tend to increase the surface concentration. Examining the P-G stability parameter for these hours, the atmosphere is neutral and the CWIC for P-G dispersion is nearly a factor of two higher than what is expected for a well-mixed boundary layer.

In comparing the CALPUFF results to Moran and Pielke's simulation, the CSU MAD model placed the maximum about 25° west of the actual plume. The statistical measures appear to be similar to the measures for the CALPUFF simulations. From Table 2, Moran and Pielke's result for the 100 kilometer arc are very similar to the CALPUFF simulation using similarity dispersion.

600 kilometers

The sampling at the 600-kilometer arc began at 0200 LST on July 9 and continued through 1100 LST on July 11. There were 20 3-hour sampling periods. The sampling began after the plume arrived at the sampling arc. The reason the plume arrived sooner than expected is discussed below. Thus, the length of time the observed plume passed the sampling monitors cannot be determined with certainty. The average observed concentrations exclude any tracer material that passed the monitors between the time the plume first reached the monitors and the time the monitors were activated. After about 1400 LST on July 9, the concentrations at the samplers were at or near background, although Ferber et al. (1981) notes that small amounts of tracer material were detected up to two days later at several of the receptors. Concentrations were simulated by CALPUFF at the 600-kilometer arc for 14 hours when using the P-G dispersion coefficients and for 13 hours when the similarity dispersion coefficients were used (Table 1). For this release and arc, 12-hour average concentrations were used for best temporal alignment with the observed data. Moran and Pielke used 15-hour simulations in the modeling of the Great Plains experiment.

The 12-hour average modeled and observed concentrations for the 600-kilometer arc on July 8 are shown in Figure 4b. Two things are apparent: 1) the observed maximum concentration is about three times higher than the simulated concentrations and 2) the maxima of the simulations are in relatively good agreement with each other.

As noted above, the tracer arrived at the sampling arc earlier than anticipated and the sampling likely missed some of the tracer material. Ferber et al. (1981) speculate that the plume probably arrived just before the samplers were activated and a small amount of plume material was not collected. The most likely reason for the earlier-than-expected arrival was the formation of a low-level nocturnal jet, supported by a variety of meteorological measurements (Moran and Pielke, 1995a). Hoecker (1963), in detailed studies of the low-level jet over the Midwestern plains (from Amarillo, TX to Little Rock, AR) using a series of pibal stations, found that jet speed maxima occur between 300 and 800 meters above local ground. In examining available data for the 1980 Great Plains field experiment, Moran and Pielke (1994) note an approximate doubling of the average nocturnal wind speeds from their daytime values. Examination of the upper air wind profiles for Oklahoma City through the period indicate the presence of a jet between 500 and 1000 meters for the 1200 Greenwich Mean Time (GMT) soundings. The wind profiles from the 1200 GMT (0600 LST) for July 8 and July 9 are shown in Figure 5. A jet of about 17 m s^{-1} is very prominent between 500 and 750 meters on the mornings of July 8 and 9. Since these soundings are taken at 0600 LST, it is possible that the low-level jet could have been stronger prior to the sounding time.

The presence of the jet is apparent in the simulated wind fields from CALMET for several periods during the night of July 8-9. Wind speed maxima are noted at levels 3 and 4 (at 50-100 and 100-500 meters, respectively) in the region of the simulated plume with noticeable drop offs in speed away from the plume. Although the input meteorology and processing in CALMET appear to have simulated the presence of a jet, the jet may not be sufficiently characterized to simulate the transport and dispersion of the observed plume. The result is a larger lateral dispersion and smaller central maximum of the simulated plumes.

Another 'feature' apparent in the simulated plume using P-G dispersion is the presence of a local maximum about 15° further east (Figure 4b). Although plume splitting was not turned on in CALPUFF, there is a definite secondary maximum. A similar phenomenon is noted in the modeling results for the 1977 INEL study by Irwin (1997) (see Figure 3c in Appendix A). The secondary maximum in the INEL study appears about 20° east of the primary maximum at the 90-kilometer arc using P-G dispersion. In both the Great Plains and INEL analyses (Appendix A), the secondary maximum is not present using similarity dispersion. A likely explanation is that the puffs became well-mixed due to greater vertical dispersion with the P-G dispersion coefficients, resulting in the puffs being affected more by the upper level winds. In examining the vertical dispersion for the first several hours after the release, σ_z for the slug or puff farthest from the source grows more rapidly to a larger value using the P-G dispersion coefficients (1400 m to 4200 m in 3 hours) compared to using similarity dispersion coefficients (1200 m to 3300 m in 6 hours). The well-mixed slugs/puffs "break away" from the other slugs/puffs and are transported by the upper level winds. In the hour before the "break away" was first noticed in the concentration pattern, the upper level winds were more from the west and the lower level winds were from the south-southwest. Figures 6 and 7 show a time series of the plume as it was transported downwind from the source, across the receptor network, and beyond using P-G dispersion coefficients and similarity dispersion coefficients, respectively. As seen in Figure 6, for 0200 on July 9 there is plume material that is beginning to be transported away from the main body of the plume. At 0700, plume material had been transported in a more westerly direction across the receptor arc and was clearly south of the main body of the plume later in the period. There was no comparable "break" when similarity dispersion was used (Figure 7).

Also of note in Figures 6 and 7 is the veering of the plume toward the east. On July 8 and 9, a large area of high pressure dominated the region. Early on July 8, a cold front associated with weak low pressure moved through the area to the southeast. The synoptic situation was such that the tracer, which was released in late morning, was transported on the western side of a this high pressure system. Moran and Pielke (1995a) show the streamline fields of the observed winds for July 8 and 9 near the surface and at about 1600 meters above ground level. The flow in the lower level is southerly and more southwesterly and westerly in the upper level, particularly later in the period.

8.2.2 July 11, 1980

Beginning at 1300 LST, tracer gases were released for a three-hour period using the same system as on July 8. The PDCH was released as an aerosol spray at an average rate of 2.41 g s^{-1}, about 1/7 the release rate on July 8. A background concentration for PDCH of 26 ppt was removed from the observed concentrations.

The samplers were set to operate for nine 45-minute periods, sufficient time for the tracer material to pass the 100-kilometer arc. The initial sampling period began at 1600 LST and continued through 2245 LST. Near-background concentrations were observed at several of the samplers for the final period (beginning at 2200 LST) and there was no report for several others for the final period. Thus, the transit time for the observed plume is six hours. The transit time of the simulated plume in CALPUFF using both P-G and similarity dispersion coefficients also was

six hours (Table 1). Therefore, six-hour average concentrations were used in this part of the analysis.

The six-hour average modeled and observed concentrations for the 100-kilometer arc are shown in Figure 8. As with the July 8 study, the monitoring did not capture the entire plume at 100 kilometers, although the peak appears to be a little better defined, with an observed maximum at receptor 18. There were no aircraft flights to assist in determining the western extent of the plume. The simulated plumes using P-G and similarity dispersion agree with each other very well, but, as with the July 8 results for the 100-kilometer arc, the peaks are more than twice the magnitude of the observed plume and the simulated lateral dispersion is less than the observed plume. The statistical measures were calculated for both the observed and simulated plumes and are shown in Table 2. Given the incomplete sampling of the observed plume at 100 kilometers for this release, the statistical measures of the observed plume likely are suspect and are not sufficient to draw conclusions regarding model performance.

Unlike the July 8 case, no aircraft observations were available on July 11 to assist in determining if the boundary layer was well-mixed. In examining "debug" output from CALPUFF, several of the slugs/puffs are well-mixed within a couple hours of the release. Comparing the simulated mixing heights to the vertical dispersion, σ_z, confirms that the boundary layer appears to be well-mixed for the daytime hours. Using the approximation CWIC = $Q/(u \bullet z_i)$ for a well-mixed atmosphere, and assuming a wind speed of 8 m s^{-1} through a mixing depth of 2600 m (from the Oklahoma City afternoon sounding for July 11), the CWIC is about 0.043×10^5 ppt-m, which is essentially identical to the observed CWIC. If the observed plume is "completed" by reflecting the rightmost three points (labeled 23, 24, and 26) on the left side, the observed CWIC becomes 0.052 ppt-m, σ_y = 16.9 km, and Cmax = 0.12 ppt.

As with the 100 kilometer arc for the July 8 study, the question remains - why do the simulated plumes have higher central maxima and narrower dispersion. A more detailed examination of the transport and dispersion algorithms in CALPUFF would be required to begin to answer this question and is beyond the scope of this effort. With a more sophisticated modeling system, Moran and Pielke (1995a,b) encountered similar differences in their examination of the July 8 simulation at 100 kilometers and could not completely explain why the dispersion model was not able to more closely represent the observed dispersion patterns at the receptor arcs.

TABLE 1

SUMMARY OF THE TIME THE PLUME ARRIVED AT THE MONITORING/SAMPLING ARCS, THE TIME FOR PLUME TO PASS THE ARCS, AND THE LOCATION OF THE PLUME CENTERLINE.

	Observed	P-G Dispersion	Similarity Dispersion	Moran Exp 4b
Arrival Time at Arc (Julian day:hour)				
Savannah River	{1}	344:1300	344:1300	--
Great Plains, July 8, 100 km	190:1545[a]	190:1600[b]	190:1600[b]	na
Great Plains, July 8, 600 km	{2}	191:0300	191:0300	na
Great Plains, July 11, 100 km	193:1645	193:1700	193:1700	--
Length of Plume Passage (hours)				
Savannah River	7-7.5	7	6	--
Great Plains, July 8, 100 km	5	6	5	3.75
Great Plains, July 8, 600 km	{2}	14	13	15
Great Plains, July 11, 100 km	6-7	6	6	--
Location of Plume Centerline (degrees from north)				
Savannah River	126	141	138	--
Great Plains, July 8, 100 km	1	357	360	17
Great Plains, July 8, 600 km	10	25	24	21
Great Plains, July 11, 100 km	15	10	10	--

{1} Sample collection starting times varied from about 10:45 a.m. to 12:30 p.m. LST
{2} Sampling started at 0200 LST on July 9 after plume arrived at the 600-km arc
[a] Starting at the 45-minute period shown (LST)
[b] For the period ending at the hour shown (LST)
na not available

TABLE 2

SUMMARY OF THE OBSERVED AND ESTIMATED CENTERLINE MAXIMUM CONCENTRATION (CMAX), LATERAL DISPERSION (σ_y), AND CROSSWIND INTEGRATED CONCENTRATION (CWIC).

		CALPUFF dispersion		Moran
	Observed	P-G	Similarity	Exp 4b
Cmax (ppt) - fitted maximum				
Savannah River	2.70	7.20	5.10	--
Great Plains, July 8, 100 km	1.30	2.70	1.90	2.34
Great Plains, July 8, 600 km	0.54	0.11	0.14	0.11
Great Plains, July 11, 100 km	0.11	0.26	0.28	--
INEL, 90 km	6.40	4.00	9.40	--
Omax (ppt) - actual maximum				
Savannah River	5.10	6.90	5.00	--
Great Plains, July 8, 100 km	1.05	2.60	1.80	2.27
Great Plains, July 8, 600 km	0.38	0.13	0.13	0.10
Great Plains, July 11, 100 km	0.11	0.25	0.27	--
INEL, 90 km	5.00	~5.30	~9.00	--
σ_y (km)				
Savannah River	11.6	7.2	6.0	--
Great Plains, July 8, 100 km	9.1	9.0	6.9	6.9
Great Plains, July 8, 600 km	19.4	64.9	42.6	28.6
Great Plains, July 11, 100 km	14.1	9.2	8.5	--
INEL, 90 km	13.1	18.9	12.3	--
CWIC (ppt-m x 10^5)				
Savannah River	0.80	1.29	0.77	--
Great Plains, July 8, 100 km	0.29	0.61	0.33	0.41
Great Plains, July 8, 600 km	0.26	0.17	0.15	0.08
Great Plains, July 11, 100 km	0.040	0.060	0.059	--
INEL, 90 km	2.10	1.90	2.90	--

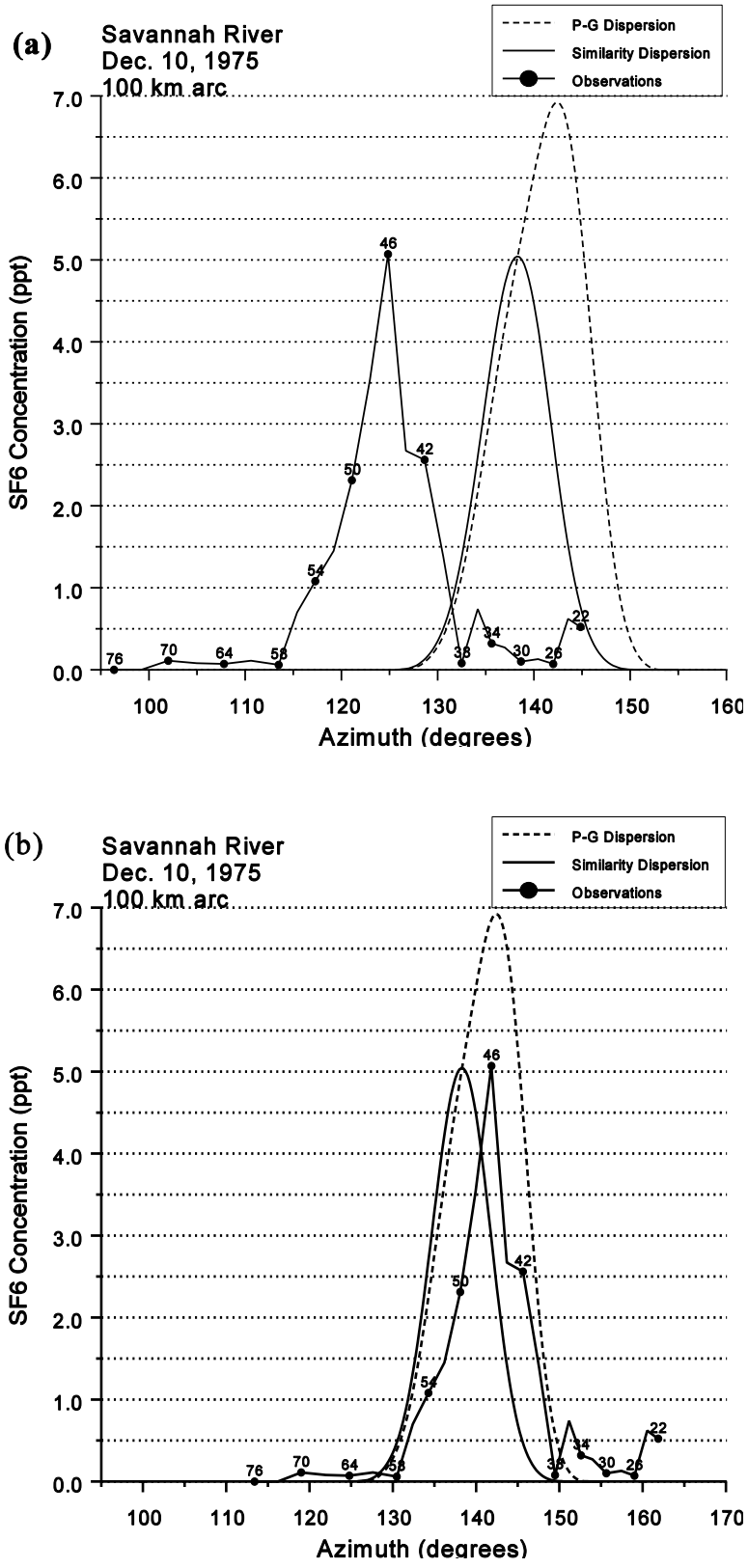

Figure 3. Simulated and observed 7-hour average plume for the Savannah River Laboratory tracer study for a) actual locations and b) observed plume offset 17° to the south.

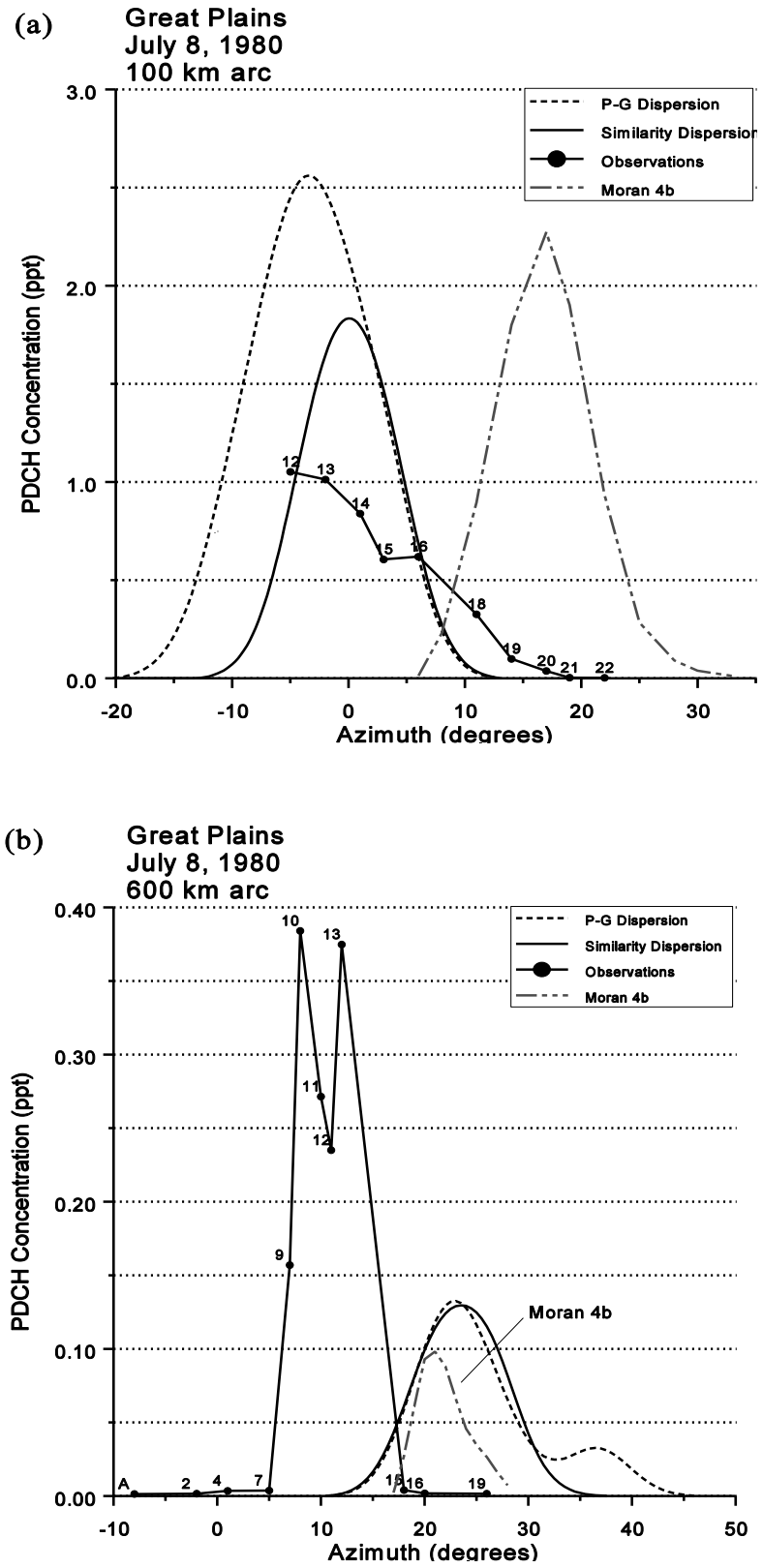

Figure 4. Simulated and observed for the Great Plains tracer study on July 8, 1980 for a) 5-hour average plume at the 100-kilometer arc and b) 12-hour average plume at the 600-kilometer arc.

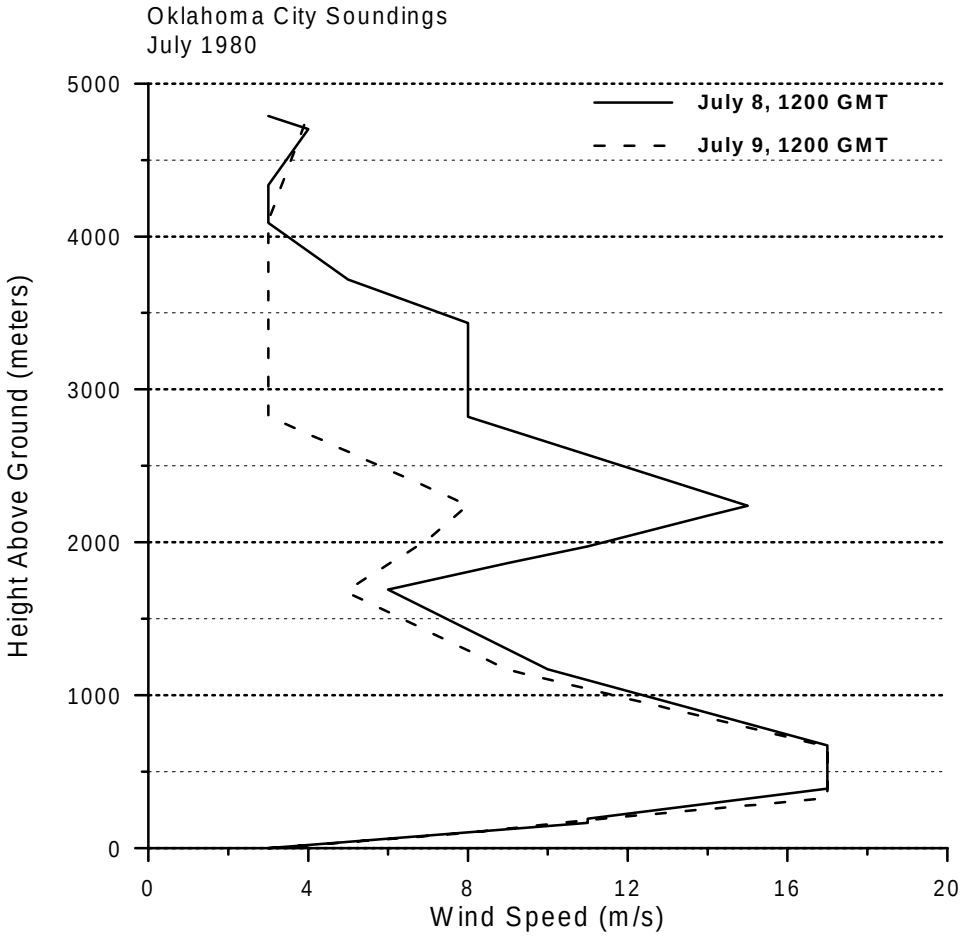

Figure 5. Upper air soundings at 1200 GMT for Oklahoma City for July 8 and July 9.

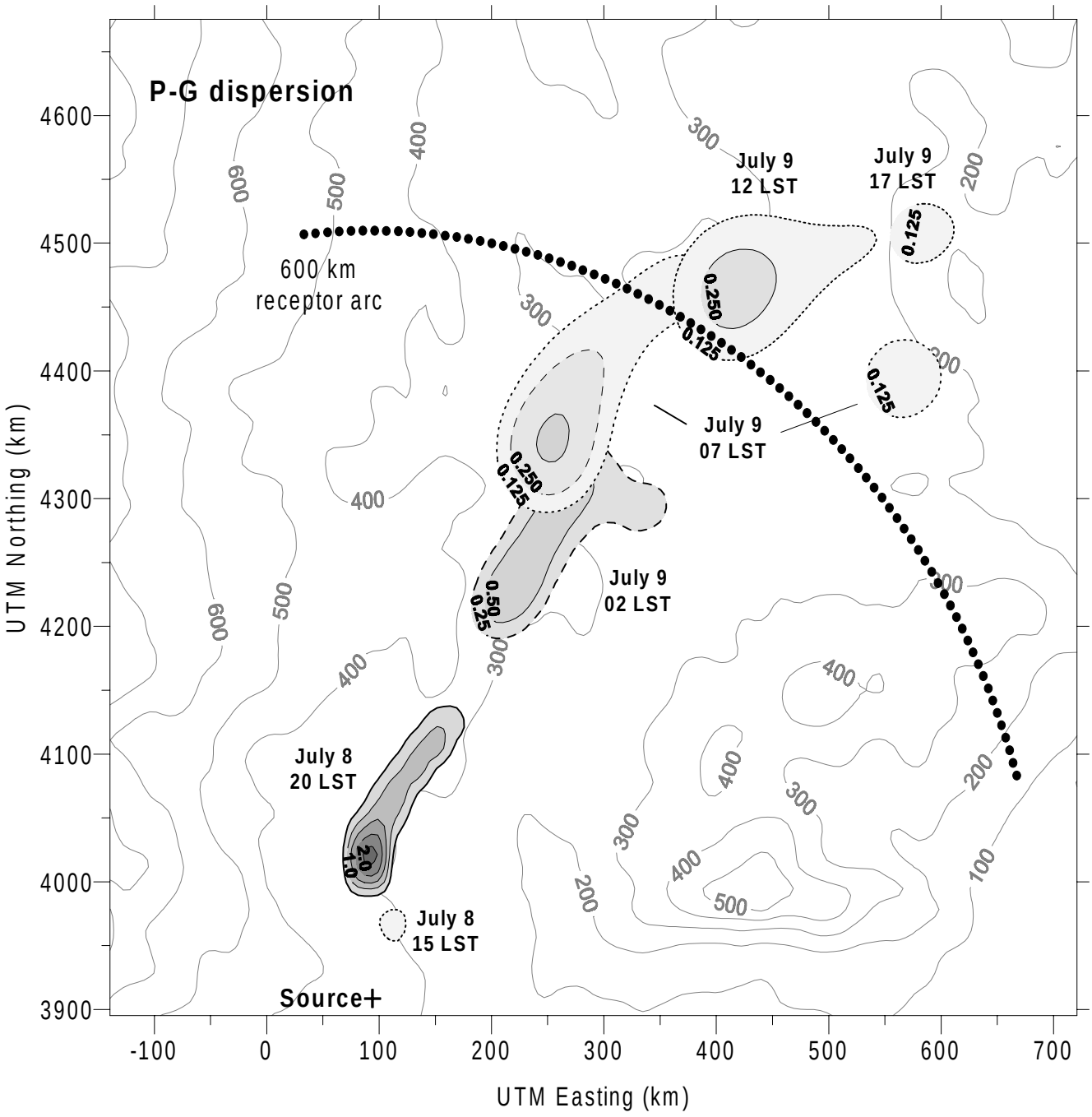

Figure 6. Location of the simulated plume using P-G dispersion coefficients for the July 8 Great Plains tracer release. Date and time are shown next to each puff. Dots are receptor locations at the 600-kilometer arc. Terrain elevations are in meters.

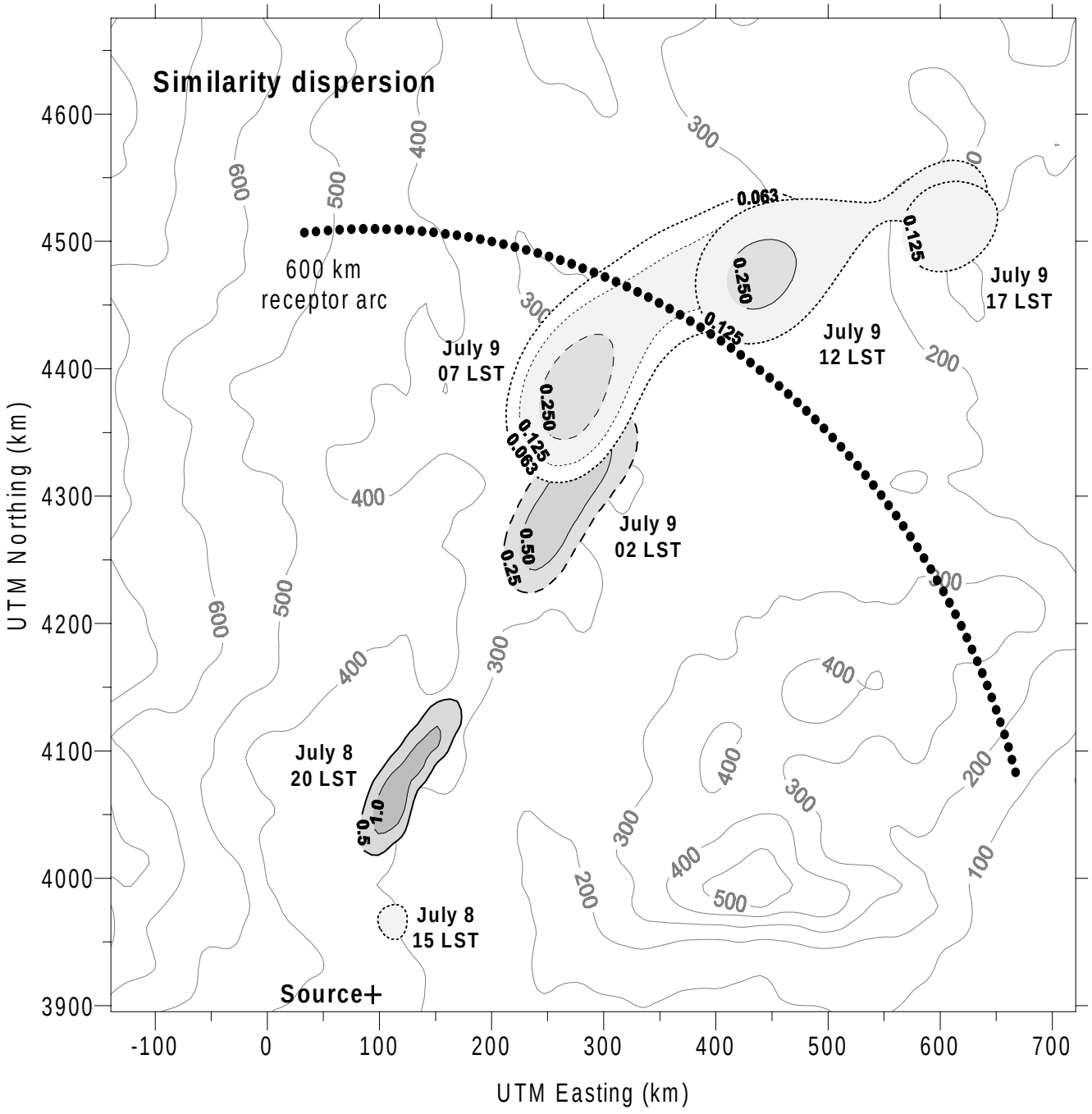

Figure 7. Location of the simulated plume using similarity dispersion coefficients for the July 8 Great Plains tracer release. Date and time are shown next to each puff. Dots are receptor locations at the 600-kilometer arc. Terrain elevations are in meters.

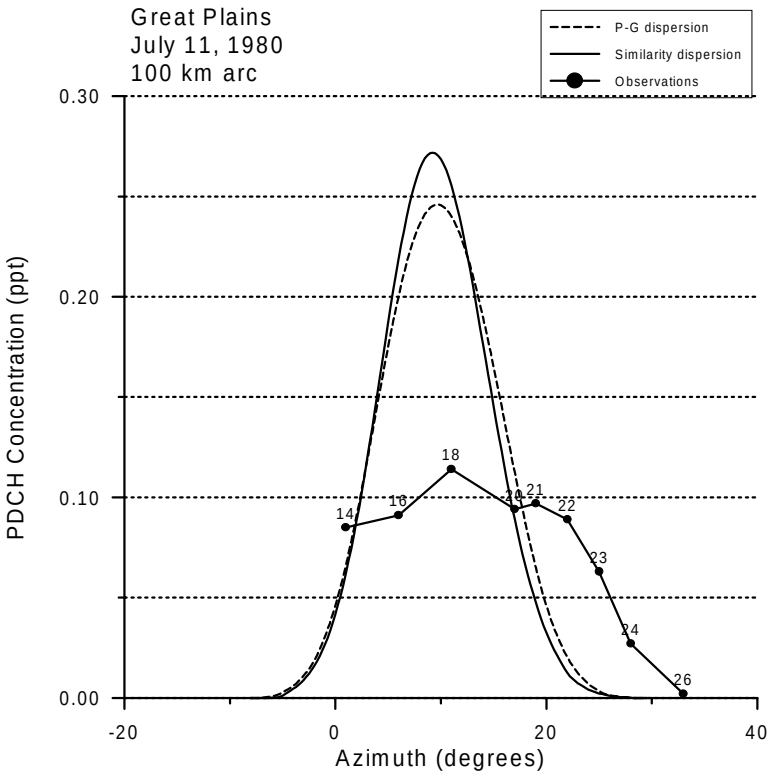

Figure 8. Simulated and observed 6-hour average plume for the Great Plains tracer study on July 11, 1980.

9.0 SUMMARY AND CONCLUSIONS

This report compares concentration estimates from the CALPUFF dispersion modeling results to concentrations observed during two long-range transport field experiments - at Savannah River Laboratory in 1975 and the 1980 Great Plains experiment. National Weather Service data and land use data with a resolution of 20-30 kilometers were used in the CALMET meteorological processor to generate the three-dimensional wind fields and other boundary layer parameters required by CALPUFF. An earlier study by Irwin (1997) examined the sensitivity of CALPUFF simulations to alternative combinations of meteorological data. Results of the baseline simulation performed by Moran and Pielke (1995a,b) using the Colorado State University mesoscale atmospheric dispersion modeling system are included for comparison to the current simulations.

For these three tracer releases, there is overall agreement between the observed times and the modeled times for both the time required for the plumes to reach an arc and the time required for the plume to pass completely by the arc. However, the transport direction tended to be off anywhere from 1° to 15°.

Most of the modeling results also can be considered in reasonable accord with the observations. The statistical measures for the simulated plumes for the Savannah River and INEL field experiments were within a factor of two of the observed plumes with no tendency for under- or overestimation. The results at the 100-kilometer arc for both study days for the Great Plains experiment consistently underestimated the lateral dispersion and overestimated the central maximum and the crosswind integrated concentration. The simulated lateral dispersion and CWIC were within a factor two of the observations, and the simulated fitted central maxima were generally 2 to 2½ times greater than the maxima fitted to the observed data. The results at the 600-kilometer arc for the July 8 Great Plains experiment show a different pattern, with the simulated CWIC and central maxima two to five times less than the observed values and the simulated lateral dispersion 2½ - 3½ times larger than the observed dispersion.

Moran and Pielke (1995a,b), using the CSU RAMS model to generate the three-dimensional wind fields and a Lagrangian particle dispersion model, encountered similar difficulties in simulating the transport and dispersion of the tracer plumes for the July 8 Great Plains experiment. As Moran and Pielke state, the Great Plains field experiment “was as simple an example of MAD [mesoscale atmospheric dispersion] as one is likely to encounter,” yet the simulations with a prognostic model and additional complexities in developing the meteorological data were no better than the simulations with the CALPUFF modeling system.

A likely reason for these differences seen in this study is that the meteorology was not adequately characterized by the CALMET meteorological processor. This is particularly true for the simulated concentrations at the 600-kilometer arc for the Great Plains experiment where the simulated lateral dispersion was much greater than the observed lateral dispersion. A likely contributor to this difference is the development of a low-level nocturnal jet on July 8 and July 9. Moran and Pielke (1995b) suggest that the most important factor for predicting the nocturnal low level jet is a realistic representation of the variability of boundary layer winds induced by the diurnal heating and cooling cycle. Thus, assumptions and simplifications in the meteorological model could also contribute to the differences seen between simulated and observed concentrations. Assumptions about atmospheric

dispersion at these larger distances in the dispersion model itself could also contribute to the differences.

The presence of the low level jet does not explain the differences seen at the 100-kilometer arc where the plume passed by the arc within four to six hours of the release. At present there is no explanation for the differences between the simulated and observed plumes.

In performing case studies such as presented here, one should keep in mind that each simulation here is only one realization of an ensemble of realizations. Turbulence, and dispersion asssociated with turbulence, is random and not predictable. Deterministic solutions are impossible. With additional observation of mesoscale dispersion, an average picture of plume transport and dispersion may be possible for the scales discussed here.

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APPENDIX A

A COMPARISON OF CALPUFF MODELING RESULTS WITH 1977 INEL FIELD DATA RESULTS

by

John Irwin

Presentation at 22nd NATO/CCMS International Technical Meeting on Air Pollution Modelling and Its Application. June 2-6, 1997. Clermont-Ferrand, France. To be published by Plenum Press in Air Pollution Modelling and Its Application XII.

A COMPARISON OF CALPUFF MODELING RESULTS WITH 1977 INEL FIELD DATA RESULTS

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INTRODUCTION

This paper provides a summary of results from a series of analyses in which puff dispersion modeling results were compared with data obtained following a single 3-hour late afternoon tracer release, lasting from 1240 to 1540 Mountain Standard Time (MST), conducted on April 19, 1977 near Idaho Falls, Idaho. The puff modeling results were obtained using the CALPUFF dispersion modeling system (EPA, 1995a,b). This modeling system consists of a meteoro-logical processor called CALMET, which is capable of developing time-dependent multi-layered wind fields using a diagnostic wind model; and a puff dispersion model called CALPUFF, which is capable of simulating the hour-by-hour variations in transport and dispersion. The tracer release results (Clements, 1979) were obtained as a consequence of an investigation into the feasibility of using certain perfluorocarbons and heavy methanes as alternative tracers in place of sulfur hexafluoride (SF6). Hence, although the results have found use for testing alternative characterizations of dispersion and transport, this was not a primary purpose in the original design of the investigation. Draxler (1979) included this experiment in an assessment of the effects of alternative methods of processing wind data for characterization of the mesoscale trajectory and dispersion. He concluded that a network of wind observations having a spacing on the order of 25 kilometers might be needed to simulate mesoscale transport associated with variable-flow situations, and that spacing of order 100 kilometers might prove adequate for stationary and homogeneous flow situations.

METEOROLOGICAL DATA PREPARATION

The design for meteorological data collection and sampling locations relative to the release location is shown in Figure 1. Since locations of towers and sites were extracted from data volume figures, the relative positions are likely accurate but the absolute positions are no

[1] On assignment to the Office of Air Quality Planning and Standards, U.S. Environmental Protection Agency

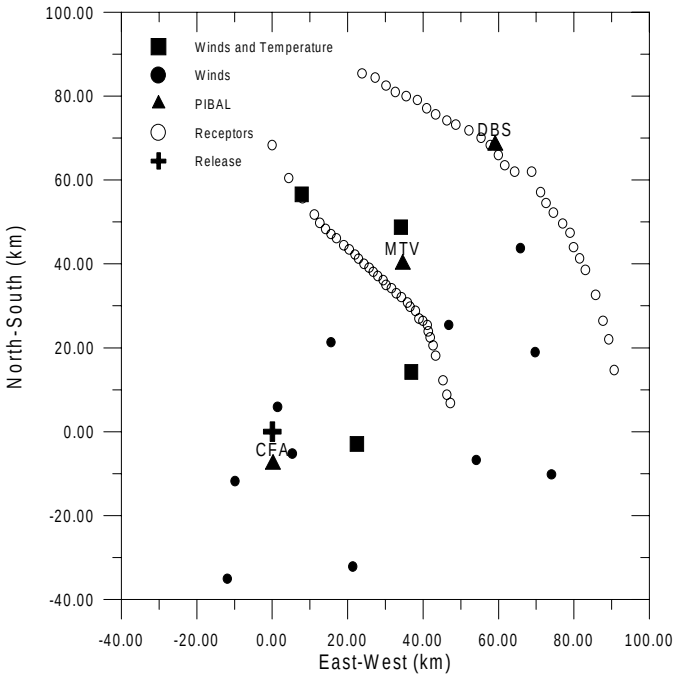

Figure 1. The Idaho tracer experiment sampling arcs and meteorological data collection network. The sampling arcs at 48 km and 90 km are shown. The receptor arc at 3.2 km downwind of the release is omitted for clarity.

better than 0.5 km. The receptor arcs at 48 and 90 km downwind from the release are shown in Figure 1. Meteorological data were available from eleven sites providing hourly-averaged winds; four sites providing hourly-averaged winds and temperatures, three sites providing hourly pibal observations of winds aloft (CFA, MTV, DBS). Two of the pibal sites (CFA and DBS) also provided hourly-averaged winds and temperatures. Hourly rawindsonde observations were taken at about 600 m northwest of the release location. The meteorological masts ranged in height above ground with two at 6.1 m, eleven at 15.2 m, three at 22.8 m, and two at 30 m. The pibal observations taken at Billings, Montana (well past the farthest sampling arc downwind) were not used in this investigation. The skies were clear of clouds and no precipitation occurred during the experiment. The National Weather Service observations taken at Pocatello, Idaho (approximately 75 km southeast of the release location) were included to provide station pressure (required input for CALMET).

To estimate the effects of drainage flow on the near-surface wind field, gridded values of land use and terrain heights are needed. The land use data are used as surrogates for typical values of surface roughness, albedo, soil heat flux, anthropogenic heat flux and leaf area index. These surface parameters are used in estimating the surface energy balance. For this analysis, U.S. Geological Service land use and terrain height data were extracted from data bases included in U.S. EPA (1996). The basic grid size for these data is approximately 900 m. They were processed into a 20 by 20 grid with a grid resolution of 10 km. Default values, as defined in U.S. EPA (1996), for the surface parameters to be associated with the land use data were used. The southwest corner of this grid was approximately 50 km southwest of the release. The area depicted in Figure 1 is fairly flat, but the terrain sharply increases in height to the west

and north of the area depicted. The dominant landuse was rangeland; and the surface roughness was estimated based on landuse to be on the order of 10 centimeters.

Hourly-averaged winds and temperature were available from midnight April 18 through midnight April 19. To mitigate the effects of not having surface data beyond midnight of April 19, the surface meteorological tower data were duplicated to form two 24-hour periods, having identical meteorology. The assumption being made is that conditions were steady-state. The pibal and rawindsonde data, which were available from 0700 MST to 1900 MST, were treated in a similar manner.

CALMET assumes all upper-air observations are from rawindsondes, and thus expects upper-air observations to provide winds, dry-bulb temperature and pressure with height. CALMET interpolates in height for missing data values at intermediate heights in an observation; but CALMET will not extrapolate upper air data. Thus observations are rejected that fail to reach the user-prescribed top of the modeling domain (3300 m for this analysis), or have missing data values at the surface. To make use of the hourly pibal observed winds, temperature and pressure values were added by linearly interpolating in time and height between available rawindsonde observations, which were available every 1 to 3 hours. The pibal wind directions were consistent with those from the one rawindsonde, but the wind speeds were generally less in magnitude.

The CALMET wind field module is based on the Diagnostic Wind Model (DWM), (Douglas and Kessler, 1988). A two-step procedure is involved in the computation of the gridded wind fields. In the first step, an initial guess field is adjusted for kinematic effects of terrain, slope flows, terrain blocking effects, and three-dimensional divergence minimization. In this analysis, the initial guess wind field varies spatially from the available upper air observations using a $1/r^2$ weighting, where r is the distance from the observation to the grid point. The second step includes four substeps: inverse distance interpolation of observations into the Step 1 field, smoothing to reduce sharp gradients in the field, adjustments of vertical velocities using the O'Brien procedure (O'Brien, 1970), and divergence minimization. In this analysis the O'Brien procedure was not used, hence the vertical velocities were not constrained to be zero at the top of the computation grid.

A purpose of this investigation was to assess the effects of having different amounts of meteorological data for use in the development of the time varying field of meteorological data. For this purpose four separate runs were made: Case 1 using all available upper-air and surface mast observations, Case 2 using all surface mast observations but only the one onsite rawind-sonde upper-air observation, Case 3 using only the CFA wind and temperature observations with the one onsite rawindsonde upper-air observations, and Case 4 using only the CFA wind and temperature observations with all upper-air observations. In Cases 1 and 2, all the onsite hourly wind and temperature data are employed but different amounts of upper-air observations are used. In Cases 3 and 4, hourly winds and temperatures taken close to the release are used with different amounts of upper-air observations. For all the CALMET simulations, winds and temperatures were computed for six layers in the vertical, the midpoints of which were: 10 m, 35 m, 75 m, 300 m, 1250 m, and 2650 m.

Figures 2a and 2b illustrate the major differences to be seen in the lowest-level wind speed and mixing heights, for the grid square containing the release. The winds at CFA were higher than those generally seen throughout the network. Hence in Cases 1 and 2 when all the onsite winds were employed (open and closed circles in the Figure 2), the low-level winds were lower than when only CFA data were used. In Cases 1 and 2, the afternoon stability was Pasquill

category B/C (Monin Obukhov lengths of order -30 m). As a consequence of higher winds in Cases 3 and 4, the surface friction velocities were higher, and the Monin Obukhov lengths were larger (in magnitude), thus closer to neutral stability. The afternoon mixing heights, shown in Figure 2b, are similar regardless of data used. This results because the "upper-air" temperatures all have a common source, namely the rawindsonde observations taken 600 m northwest of the release. The nighttime mixing heights are mostly a function of the magnitude of the friction velocity. Hence, where estimated friction velocities were largest and differ most among the various processing methods, differences were to be seen in the nighttime mixing height values (see hours 1800 to 2300 MST in Figure 2b).

DISPERSION MODEL CALCULATIONS

Each of the four analyses of meteorology was used to produce two CALPUFF simulations of ground-level concentrations for each of the three sampling arcs. In the first simulation, the dispersion was described using Pasquill-Gifford dispersion parameters. In the second simulation, the dispersion was described using dispersion parameters suggested by Draxler (1976), which require values of the standard deviation of the vertical and lateral wind fluctuations (referred to hereafter as "similarity dispersion"). The wind fluctuation standard deviations estimated within CALMET are primarily dependent on the surface friction velocity. The surface friction velocity is a strong function of stability (largest during unstable conditions), roughness length and wind speed (increases as roughness length or wind speed increase). The CALPUFF user's guide (EPA, 1995b) provides a complete listing of the various equations, which is not possible to provide in this limited discussion.

CALPUFF options were set as follows: the maximum puff travel distance during one sampling step (controls the puff generation rate) was set to 1 km, maximum puff separation was set to 1 km, Gaussian vertical distribution was assumed, concentrations were determined as if over flat terrain, no wet or dry deposition, and no transition to Heffter long-range dispersion parameters was made.

CALPUFF internally computes for each sampling step, a transport wind averaged over the depth of the puff from the multi-layer winds provided to it from CALMET. As a surface release puff grows in the vertical, the depth through which the wind is averaged increases. The SF6 tracer emission was reported to be steady at 25.37 gs^{-1} over the three hour period, and was simulated within CALPUFF as a 3-hour point-source release at 10-m starting at 1300 MST. The release height was set at the midpoint of the lowest CALMET layer, to insure that the internally computed standard deviations of lateral and vertical velocity fluctuations (for use in the similarity dispersion parameter characterizations) at the specified release height, were in accord with the wind speed used by CALPUFF for the lowest layer.

MEASUREMENT UNCERTAINTIES

The primary sampler used in this experiment was a bag sampler, consisting of a 50-liter Saran bag enclosed in a plastic barrel. The bag was inflated with a small battery-powered pump, which was turned on and off manually In general, 6-hour samples were available with approximate start times of 1200 MST on the 3.2-km arc, 1300 MST on the 48-km arc, and 1500 MST on the 90-km arc. Two aliquot samples were taken from each bag, one into a 2-liter bag and the other into a 1-liter steel cylinder. Of the 68 valid SF6 concentration values

reported, 48 were from cylinder samples. For the 17 occasions where SF6 concentrations from both the bag and cylinder samples could be compared, the bag samples were consistently 37% lower than the cylinder samples. No discussion was present in the data volume regarding these differences between the bag and cylinder samples, but all plots were shown using the cylinder samples. In light of this and the differences seen between the bag and cylinder samples, only the cylinder concentrations were used in the following analyses. To estimate the sampling uncertainty in the SF6 cylinder samples, comparisons where made with the three perfluorocarbons which were released simultaneously at the same location with the SF6: PDCH (C_8F_{16}), PDCB (C_6F_{12}), and PMCH (C_7F_{14}). Comparison of SF6 concentration values with concentrations from cylinder samples from all three perfluorocarbons was possible at 33 sites along the three sampling arcs. The perfluorocarbon concentration values were found to be consistently 14% greater than the SF6 concentrations. For SF6 concentrations greater than 20 ppt, the standard deviation of the percentage differences was 11%; and for SF6 concentration less than 20 ppt, the standard deviation of the percentage differences was 77%, implying greater uncertainty for the lower concentration values. A background of 0.5 ppt was subtracted from all SF6 concentration values as suggested in the data volume.

MODEL RESULT COMPARISONS

For each 6-hour period, the second moment (lateral dispersion, Sy) of SF6 concentration values about its centroid position along the arc was computed. The crosswind integrated concentration, CWIC, was computed by trapezoidal integration. By assuming the concentration profile along the arc is Gaussian, the central maximum, Cmax, was computed as,
$Cmax = CWIC/(\sqrt{2\pi}\ Sy)$.

A goal of this investigation was to assess the sensitivity of the modeling results to different treatments of processing the meteorology, as well as to assess the performance of CALPUFF in characterizing dispersion for transport distances beyond 50 km. Results are summarized in Table 1 for the different wind field and dispersion treatments. Figure 3 depicts the observed SF6 concentrations with the simulation results where all the surface and upper-air observations were used to generate the hourly wind fields. For the observed values, there were from 14 to 17 receptors along each arc with valid data for analysis. For analysis of the simulation results, receptors were spaced at each arc distance at 2 degree intervals, over the 90 degree sector northeast of the release location. The second moment, Sy, represents a measure of the puff horizontal dispersion. For these 6-hour periods, the observed lateral dispersion ranged from roughly 22% to 15% of the travel distance downwind. The crosswind integrated concentration values characterizes the amount of pollutant mass seen at the surface. From Figure 2, assuming a mixed layer wind speed of 4 m/s, a mixed layer depth of 2500 m, a sample duration of 6 hours, we would anticipate CWIC values of approximately $2x10^5$ ppt-m, if the puff was well mixed. The observed CWIC values at 3.2-km and 90-km arcs are close to $2x10^5$ ppt-m. The CWIC value at 48 km, shown in Table 1 as $4x10^5$ ppt-m, would be $2x10^5$ ppt-m, if we assumed the observed concentrations beyond receptor 425 rapidly approached zero. There are indications of such a falloff in concentration in the bag sampling results, but only the cylinder results shown in Figure 3 where analyzed in developing Table 1.

As shown in Figure 3 (which is typical for all of the simulations), the simulated transport was somewhat south of the observed position along the first two arcs. It is also apparent that the concentrations simulated for the first arc are at least a factor of 5 higher than observed.

Table 1. Summary of observed and estimated centerline maximum concentration, Cmax, lateral dispersion, Sy, and crosswind integrated concentration values, CWIC.

	Pasquill Dispersion			Similarity Dispersion		
Cmax (ppt)	3.2 km	48 km	90 km	3.2 km	48 km	90 km
Observed	103	16.6	6.4	103	16.6	6.4
All SFC + All UA	793	11.4	4.0	945	21.0	9.4
All SFC + 1 UA	808	9.8	2.5	955	20.0	5.4
1 SFC + 1 UA	1903	25.2	12.5	896	10.0	5.9
1 SFC + All UA	1712	27.2	12.0	854	17.1	8.6
Sy (km)	3.2 km	48 km	90 km	3.2 km	48 km	90 km
Observed	0.70	9.66	13.06	0.70	9.66	13.06
All SFC + All UA	0.46	5.22	18.93	0.66	5.31	12.27
All SFC + 1 UA	0.46	5.15	13.66	0.66	5.27	8.43
1 SFC + 1 UA	0.30	4.79	5.76	0.55	4.38	5.38
1 SFC + All UA	0.37	4.67	9.21	0.60	4.35	9.31
CWIC (ppt-m x 10^5)	3.2 km	48 km	90 km	3.2 km	48 km	90 km
Observed	1.82	4.02	2.09	1.82	4.02	2.09
All SFC + All UA	9.17	1.50	1.88	15.63	2.79	2.88
All SFC + 1 UA	9.21	1.27	0.87	15.67	2.58	1.15
1 SFC + 1 UA	14.22	3.03	1.81	12.31	1.10	0.79
1 SFC + All UA	15.89	3.18	2.78	12.91	1.86	2.01

There is no obvious reason to dismiss the 3.2-km observations, as the other tracers at this arc were within 11% of those reported for the SF6 when adjusted for differences in release rates. The differences seen in the different treatments to develop the wind fields can largely be explained by the increase in the lower level winds by a factor of 2 when only the winds at CFA are used to develop the wind fields. As the transport winds increase, not only was the transport to the arc decreased, but also the variability in the wind directions within the wind field were greatly reduced. The transport time to the 3.2 and 48 km arcs varied from 1.5 to 3 hours, depending on meteorology used. With these transport times and 10-km meteorology, the lateral dispersion is relatively insensitive to the meteorology used for the 3.2 and 48 km arcs. The CWIC values vary inversely to the product of the simulated vertical dispersion and the

mean transport speed. For the Pasquill results, an increase in wind speeds results in neutral stability, which caused the vertical dispersion to be nearly a factor of 4 less. This more than compensated for the increased dilution, hence higher CWIC values. For similarity dispersion, the vertical dispersion was never well-mixed and was nearly the same, regardless of meteorology used. Beyond 75 km, an increase in transport winds tended to increase the simulated vertical dispersion by 30% or so, which tended to reduce CWIC values for the 90-km arc.

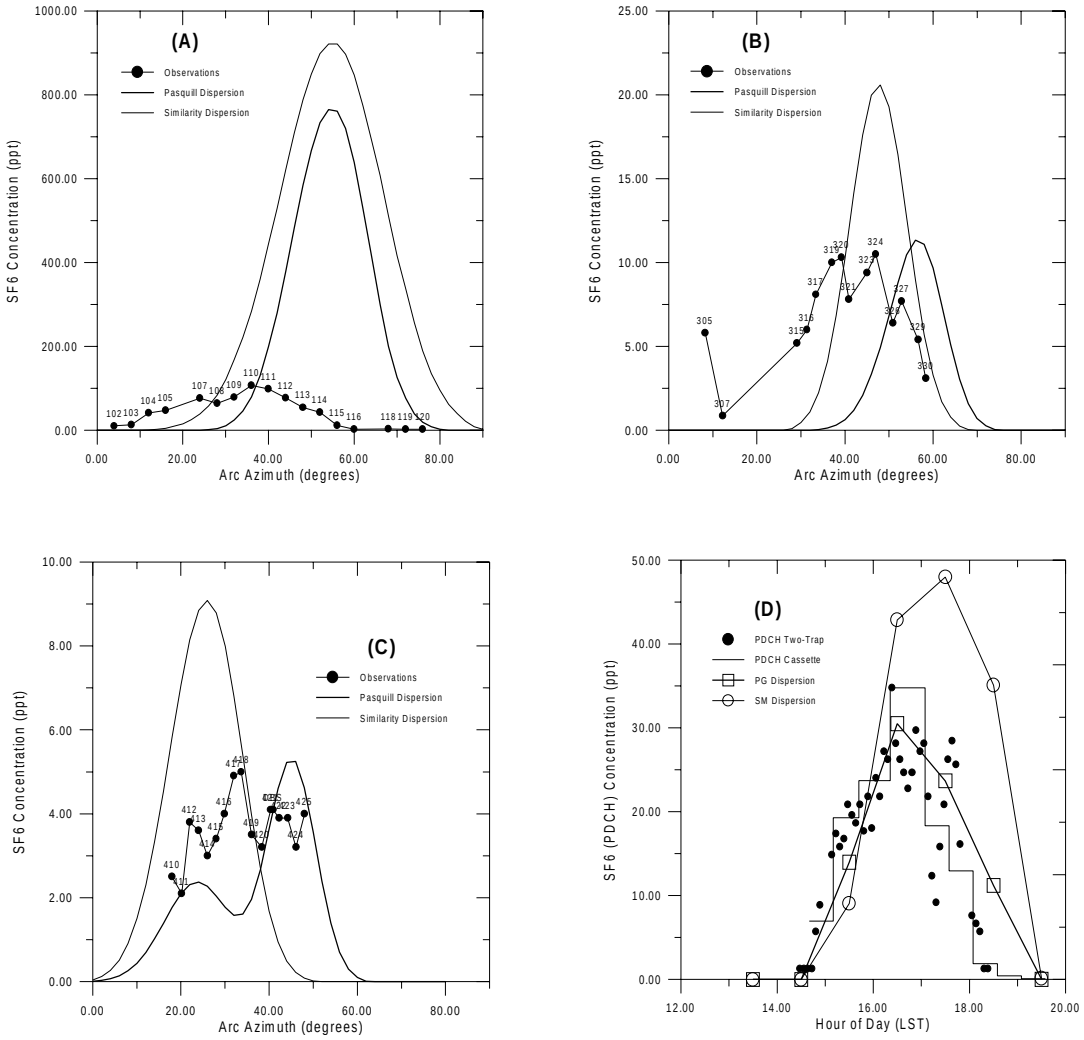

Figure 3. Six-hour average SF6 concentration values observed and estimated for April 19, 1977, (A) 3.2-km arc, 1300-1900 MST; (B) 48-km arc, 1400-2000 MST; (C) 90-km arc, 1600-2200 MST. Azimuth is defined as viewed from the release position with 0 due North and 90 due East (see Figure 1). Receptor numbers are shown just above each observed concentration value. (D) Time history of observed PDCH and estimated SF6 concentrations along the 48-km arc for April 19, 1977. Observed PDCH values were multiplied by 3.16 for comparison with estimated SF6 values (volume of SF6 divided by volume of PDCH released equals 3.16).

Figure 3d provides a comparison of the time history of the puff, as it passed by the 48-km arc. Sampling results are shown for the two-trap sampler which provided 5-minute samples, and a cassette sampler which provided approximately 15-minute samples. These samplers were quite close to the observed position of the 6-hour SF6 maximum along this arc. The dispersion results are for the simulated position of the maximum, which was somewhat displaced from that observed. The Pasquill dispersion results are in remarkable accord with the tracer results. The similarity results arrive and depart slightly later than observed. The slower transport for the similarity dispersion results because the vertical dispersion was less than that simulated by Pasquill dispersion, hence the transport speed was computed over a more shallow layer for the similarity results. These results and those discussed above suggest that the similarity dispersion was underestimating the vertical dispersion for this case.

CONCLUSIONS

A goal of this investigation was to assess whether the CALPUFF simulations were in reasonable accord with the observed concentrations, and the sensitivity of the simulation results to different methods of processing the available meteorological observations. The comparison results presented reveal as yet unexplained differences for the nearest arc, 3.2 km downwind from the release. Possible speculations are that the puff became well-mixed sooner than we would otherwise expect, or that the puff lifted somewhat off the surface at the 3.2-km arc. The simulated pattern of dispersion was displaced as much as 40 degrees from that observed, regardless of how the wind fields were characterized. For all arcs, the lateral dispersion along the sampling arcs was best characterized by both dispersion characterizations when all the surface tower winds were used. Except for the first sampling arc, the simulated maxima along the arcs were typically within a factor of 2 of that observed. The Pasquill simulations were most sensitive to how the wind fields were characterized, showing the most variability between the various wind field results. Having only one puff release limits conclusions to be reached. For this one realization, it would appear that simulations by both dispersion characterizations were in best accord overall with observations when all the low-level winds and upper-air observations were used. And for this case, the similarity dispersion simulations may have underestimated the vertical dispersion.

DISCLAIMER

The information in this document has been funded wholly or in part by the United States Environmental Protection Agency under an Interagency Agreement (DW13937039-01-0) to NOAA. It has been reviewed in accordance with the Agency's peer and administrative review policies for approval for presentation and publication. Mention of trade names or commercial products does not constitute endorsement or recommendation for use.

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APPENDIX B

COMPACT DISCS

Solar and Meteorological Surface Observation Network (SAMSON), 1961 - 1990
Version 1.0, September 1993

Available from U.S. Department of Commerce, National Climatic Data Center, Federal Building, 151 Patton Avenue, Asheville, NC 28801

Radiosonde Data of North America, 1946 - 1992
Version 1.0, August 1993

Available from U.S. Department of Commerce, National Climatic Data Center, Federal Building, 151 Patton Avenue, Asheville, NC 28801

CALMET, CALPUFF, and CALPOST Modeling System
Version 1.0

Available from U.S. Department of Commerce, National Technical Information Service, 5285 Port Royal Rd. Springfield, VA 22161. NTIS PB 96-502 083.

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16. ABSTRACT

The performance of the CALPUFF atmospheric dispersion model for two field tracer experiments is summarized. The first tracer experiment was in 1975 at Savannah River Laboratory and the second was in 1980 in the central United States. Both experiments examined long-range transport of an inert tracer material. The results generally were encouraging, with the simulated results within a factor of two of the observed data for the statistical measures presented in the report. However, there is not a consistent pattern of over- or under-estimation relative to the observations.

17. KEY WORDS AND DOCUMENT ANALYSIS

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CALPUFF Regional Modeling Air Dispersion Models	Tracer Experiments Model Performance Long-Range Transport	

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